Density Due to Collective versus Fluctuation Kinetic Energy in Classical, Classical Statistical and Quantum Mechanics

Francesco R. Ruggeri Hanwell, N.B. Jan. 2, 2019

The purpose of this note is to consider spatial densities in the case of classical mechanics (1/v), quantum mechanics (W(x)*W(x) for bound states) and statistical mechanics exp(-V(x)/T) with respect to the effects of collective motion. In the classical mechanical case, with a density of 1/v, the entire motion is collective and seems to be modeled as a compressible gas with flux continuity. (It seems that this idea may even possibly lead to Newton´s second law.) In the case of quantum mechanics, high energy eigenvalue densities are supposed to approach the classical density near peak density points. We try to investigate why by considering root mean square velocities and what we think is fluctuation flux in a quantum system. For peak wavefunction values dW(x)/dx=0 and we try to show that these points represent places where there is no fluctuation flux. Thus, at such points, there is only collective motion and one would expect W(x1)W(x1) vave(x1) =W(x2)W(x2) vave(x2) between two such points x1 and x2, i.e. a continuity equation. For points in between, fluctuation flux mixes with collective velocity to create a more complicated pattern. In such high energy cases, cycling time 1/E from exp(iEt) is small, so the idea of a density at a point x at a time t with a small delta t seems to make sense. Actual results of the intersection of 1/v(x) and the quantum density are not actually at the peak, but the peak seems to be the approximating the match. (3)
For low quantum energies, the cycling time 1/En is long compared to times required to traverse the system and fluctuation flux mixes with collective motion. For the quantum oscillator this leads to a Gaussian. We also examine the case of the classical statistical oscillator and argue that the fluctuation flux (the thermal kinetic energy) is mixed with collective kinetic energy which leads to higher interparticle spacing for places where the potential is higher.

Classical Mechanics

In general, classical mechanics can be described using Newton´s second law. In such a case, one usually consider a tiny fixed delta t interval and determines different delta x intervals for different velocities. It is possible, however, to consider a fixed delta x interval and calculate different delta t intervals to obtain the same velocity as velocity is a ratio of delta x / delta t. The reason to maintain a constant delta x interval is that one may wish to deal with densities. In such a case (one dimensional), the density d(x) is multiplied by a fixed delta x, forcing delta t to vary. In (1), it was suggested that for a classical particle in a potential, the density d(x) was equivalent to dt =dx/v(x) with dx being constant and dt varying with x. v(x) is then calculated from v(x)= sqrt(2m(E-V(x)) where V(x) is the potential. It was suggested in (2), that one could obtain the same result using d(x1) v(x1) = d(x2) v(x2) i.e. a continuity of flux equation. Let us examine this in more detail. Consider Newton´s second law:

F=dp/dt = mdv/dt + dm/dt v

In general, dm/dt is zero, but if one is considering fixed delta x units and different velocities in each, one can have a density which changes in time. If cross-sectional area and delta x are fixed then dm/dt = area delta x d d(x)/dt. If d(x)=1/v as suggested above, then F=0, i.e. one has a compressible gas which moves subject only to internal forces involved in compressing it and changing its velocity. In fact, one has equal and opposite forces for F=0, which seems to be action/reaction. Thus, normally one considers m=constant delta t = small constant and deals with different delta x values. Next, one considers delta x = small constant with a varying delta t. As a third step, one considers density varying with x and external force disappears altogether.

The reason for belabouring some ideas behind a density d(x)=1/v for a classical particle is that in the large energy limit, quantum mechanical density is supposed to approach this classical density (or at least an asymptotic envelope on the quantum mechanical density approaches it (3)).

Quantum Mechanics

In quantum mechanics, one calculates a wavefunction W(x) and energy eigenvalues from a time-independent Schrodinger equation for bound states. The density is Wn(x)Wn(x) for any energy eigenvalue En. It should be noted, however, that there is cycling in the wavefunction as the time-dependent factor of the wavefunction is exp(iEnt). Thus, there is a frequency En and a characteristic time 1/En (up to an hbar factor). Even though a density is defined for all En, for small En, the time 1/En may be of the order of the time taken to traverse the entire bound region. For example, for an oscillator with mechanical frequency w, low energy levels are of the same order as w, so it does not seem to make sense to think of the density Wn(x)Wn(x) as existing at a particular point x at a time t plus delta t. As En becomes large, however, 1/En, the cycling time becomes very small compared to the time required to traverse the bound region and Wn(x)Wn(x) is not just a spatial density average over a long time.

It seems that in quantum mechanics, interference is essential. This interference occurs between different ¨ sine waves¨ during the cycle time 1/En. The interference creates the wavefunction value at a point x and hence the density and also the kinetic energy density i.e.

W(x) = Sum over p fp sin(px) and Kinetic energy density = W(x)[Sum over p p*p/2m fp sin(px)] Here fp is the weight of the momentum p (or the Fourier component weight).

In quantum mechanics, collective flow is supposed to correspond to a complex wavefunction. A bound wavefunction, however, is real. It is known that there is a kinetic energy density so there is motion. Furthermore, at each point x, there is a root mean square velocity from the classical energy conservation equation: .5m v(x)*v(x) + V(x) = E. This is still valid in the quantum mechanical scenario and perhaps represents a kind of collective velocity.
One can also write: i d/dx W(x) = i Sum over p fp p cos(px). This is not zero implying that there is some kind of momentum flux perhaps due to fluctuations in the bound state. Consider the case of a quantum harmonic oscillator. As En becomes large, the wavefunction contains ¨humps which decrease in height as one moves toward x=0 and then increase again. The top of

each hump corresponds to d/dx W(x) = 0. Each point on the wavefunction graph corresponds to a density W(x), a time t (with a delta t of the order 1/En) and a v ave(x) where v ave(x) is the classical velocity. Now W(x1)W(x1) v ave(x1) is general not equal to W(x2)W(x2) v ave(x2). It is argued (3) that the equality only holds near the top of humps. At these tops we argue the flux due to fluctuations is zero. At such points there is only collective velocity given by v ave(x) it seems. Thus, the flux continuity equation W(x1)W(x1) vave(x1) = W(x2)W(x2) vave(x2) only applies at these points. Thus, even in the high En limit, quantum mechanics only approximates classical mechanics at certain points. It seems that these points (at least for the oscillator) increase as En increases, but quantum mechanics still remains a theory of resonance. In (4), it was argued that one has 2x2 matrix type particles which bounce back and forth while only moving on average with v in one direction. Thus, v is a kind of collective motion, while there is other motion occurring internally. Quantum mechanics is a resonance of these 2x2 matrix particles, it is argued, and is also a resonance type theory. The term exp(iEt) of a bound state describes the internal resonance. Only at peak points in the wavefunction does the collective velocity vave(x) appear without fluctuations, allowing for a density times collective velocity description and even this seems to only make sense for high En so that 1/En, the cycling time of the resonance is very small so that the density at a point can be established at time t with a very small delta t.

For the quantum oscillator ground state, the energy is related to the mechanical frequency showing an apparent link between collective classical motion and the quantum resonance. The problem is that the two are of the same order, so that the quantum cycling takes as long as a mechanical oscillation. Thus, even though there is a density W(x)W(x), where W(x) is a Gaussian in space, it seems that the averaging necessary to calculate this density takes so long that one cannot consider conservation of flux W(x)W(x) vave(x) at all.
There is only one point, x=0, where d/dx W(x)=0, so there seems to be flux due to fluctuations everywhere else and these are mixed in with the collective motion of the oscillator so that it cannot really be seen except through the fact that the ground state energy is proportional to mechanical oscillator frequency and the following form of the Schrodinger equation:

[Sum over p p*p/2m fp sin(px)]/W(x) + V(x) = E ((1))

This holds for any E eigenvalue including the ground state, with the first term being the average kinetic energy which equals the classical value .5m vave(x)^2.It seems, however, that it takes a long time (1/Eground state), for this average to be taken, i.e. for cycling through the various p (momentum) values. The fact that there is a V(x), creates a v ave(x) in the first place, but it seems to be intertwined with fluctuation flux and so the density does not resemble the classical 1/v(x) at all. In fact, it is the opposite.

Classical Statistical Mechanics

For the case of a classical statistical mechanical oscillator, the spatial density is Gaussian, as in the ground state of the quantum oscillator. In addition, the fp values of ((1)) are equal to exp(-ap*p), with a being a constant, which mimics the momentum distribution of the oscillator.

Again, as in the quantum case, there should be collective motion intertwined in the various thermal motion. It is the potential V(x) which is responsible for the spatial density and this potential is also responsible for collective motion which is occurring in both directions at the same time. Again, it might take quite some time to measure classical statistical mechanical averages. For example, consider an oscillator potential between two walls. Imagine that particles at each wall have only thermal energy and that the gas is sparse.
If one starts with a Boltzmann distribution in velocity at one wall at time t, the particles have different speeds and will arrive at the second wall at different times. Thus, it does not seem that having all particles of the Boltzmann distribution arriving at a wall at the same time is an equilibrium scenario. If that is the case, it will take some time (relative to the average time to cross the system) for one to measure the velocity distribution.

In a classical statistical system, there is a constant temperature everywhere, thus there is thermal energy or fluctuation energy everywhere at the same time there is collective velocity due to the potential. Due to the predominance of the fluctuation energy, with particles in different locations with different velocities, the effect of the collective velocity or potential it seems is to change the density from the constant value it would have in the absence of the potential. As a hand-wavy example consider two particles moving in the same direction and then two particles moving in opposite directions in a small time interval dt.

In the absence of a potential, each particle would move vi dt where vi is the velocity. For the case of a constant acceleration -dV/dx in a tiny time interval dt, each particle would move vi dt $-.5/m\ dV/dx\ (dt)^2$. The extra distance due to the potential is velocity independent and does not affect particles moving in the same direction. For particles moving in opposite directions, however, the interparticle separation is increased and this is related to dV/dx. Thus, one would expect lower densities in regions with high dV/dx. For an oscillator, the end regions would have low density and the central high which is qualitatively similar to the Gaussian result. Again, it is difficult to sense any collective motion as it affects the density, but it seems to be there and seems to be similar to the fluctuation flux in the quantum oscillator case.

Conclusion

In conclusion, it seems that quantum mechanical and classical statistical mechanical systems contain both collective and fluctuation kinetic energies that mix. In such a case, the collective kinetic energy, due to the presence of a potential V(x), seems to create a spatial density. In the case of the oscillator, the density is low in places where V(x) is high. For the quantum case, as energy eigenvalues increase, not only does the cycling time increase (leading to the idea that density can be measured at a time t with a small delta t at a point x), but peak points d/dx W(x), where W(x) is the wavefunction, seem to be places where there is no fluctuation flux. In such a case, there is a well defined density at these points and only collective kinetic energy and so a flux continuity equation W(x1)W(x1)vave(x1) = W(x2)W(x2)vave(x2) seems to apply. In the case of classical mechanics an identical equation seems to hold leading to density = 1/v(x) where $.5m\ v(x)^2 + V(x) = E$.

References

1 Majernick V and Opatiny Y. Entropic uncertainty in classical quantum Oscillator (J Phys A Math Gen, 1995, UK) http://www.ktf.upol.cz/tom/clanky/jpa96-ent.pdf
2 Ruggeri, Francesco R. Possible Relation Between Quantum Mechanical Cycling Exp(iEt) and the Correspondence Principle and Physical Oscillating Objects Like Phonons and Photons (preprint, zenodo, 2018)
3 http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc6.html
4 Ruggeri, Francesco R. The 2x2 matrix model and the Schrodinger Equation (preprint, zendo, 2018)